UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
CENTER FOR ENVIRONMENTAL MEASUREMENT AND MODELING
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OFFICE OF
RESEARCH AND DEVELOPMENT

September 24, 2020

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Subject: NJ DEP Data Report #8: Non-targeted Analysis of PFAS in Water Samples

Dear Mr. Kloo:

I am pleased to provide you with the attached laboratory report that includes non-targeted analysis (NTA) results for per- and polyfluoroalkyl substance (PFAS) in water samples collected from tidal and non-tidal surface water and groundwater wells. This is the eighth in a series of reports prepared as a part of EPA Office of Research and Development's (ORD) collaboration with the New Jersey Department of Environmental Protection (NJ DEP) and EPA Region 2 on the study, "Detection, Evaluation, and Assignment of Multiple Poly- and Perfluoroalkyl Substances (PFAS) in Environmental Media from an Industrialized Area of New Jersey." We previously reported targeted analysis results for these same samples (NJ DEP Report #3 dated April 17, 2019).

It is our understanding that this study was designed to help NJ DEP in your ongoing investigation into the presence of PFAS in the environment near manufacturing facilities of interest. This study relates to our research capabilities and interests applying targeted and non-targeted analysis methods for discovery of the nature and extent of PFAS environmental occurrence that may be potentially associated with industrial releases. EPA continues to develop analytical methods for many PFAS compounds in various media, including some of those included in this report. We are providing the results of our analyses as they become available.

In this report, we provide tentative identification and semi-quantitative analytical results for 47 PFAS. We do not interpret exposure or risk from these values. EPA does not currently have health-based standards, toxicity factors, or associated risk levels for PFAS, other than perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), and perfluorobutanesulfonic acid (PFBS). While the data provided in the attached report indicate the presence of PFAS in the water samples, we do not have sufficient information to offer interpretations related to human or environmental exposure and risk.

Thank you for inviting us to be part of this effort that helps to further both EPA's and New Jersey's understanding of an important issue in the state. This is just one of many Agency efforts that demonstrates EPA's commitment to working with our state partners.

If you have any questions or concerns about this report, do not hesitate to contact me at (919) 541-5114 or via email at Watkins.tim@epa.gov. I look forward to our continued work together.

Sincerely,

Timothy H Watkins

Timothy H. Watkins
Director

Enclosure

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Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey

Laboratory Data Report #8: Non-targeted Analysis of PFAS in Water Samples Collected from Tidal and Non-tidal Surface Waters and Wells

Background. This report is a product of a collaborative study with EPA ORD, EPA Region 2, and NJ DEP entitled "Detection, Evaluation, and Assignment of Multiple Poly- and Perfluoroalkyl Substances (PFAS) in Environmental Media from an Industrialized Area of New Jersey". NJ DEP assumed responsibility for the collection of samples and their shipment to the ORD laboratory in Research Triangle Park, NC. ORD was responsible for sample extraction and analysis of PFAS. Sample analysis and preparation of this report involved many from ORD assuming various roles and responsibilities (Table 1).

Table 1. EPA Office of Research and Development Lab Analysis and Report Team.

Responsibility	Personnel
ORD Principal Investigators	Andy Lindstrom, Mark Strynar, and John Washington
Laboratory Chemistry Analysis	Mark Strynar, James McCord
Quality Assurance Review	Sania Tong Argao, James Noel
Management Coordination and Review	Myriam Medina-Vera, Brian Schumacher
Report Preparation	Kate Sullivan

This 8th report includes non-targeted analyses (NTA) results for 74 water samples, including unknowns, field duplicates, and field blanks, collected from tidal and non-tidal surface waters and groundwater wells. Sample collection was the responsibility of NJ DEP and primarily occurred between October 17 and December 7, 2017. Samples were shipped to ORD on several dates between November 3 and December 15, 2017. Several additional groundwater well samples, plus a duplicate sample, were received by ORD outside this timeframe and these results are also included. The samples were analyzed for PFAS under the direction of Dr. Mark Strynar at ORD's laboratory in Research Triangle Park, NC.

This report complements NJ DEP Report #3[1] where ORD provided quantitated results for 10 PFAS using targeted analysis for the same water samples. This 8th report provides results for additional PFAS compounds uniquely identified by NTA. Previously quantitated PFAS analytes that were also detected with NTA (e.g., PFOA) are *not* included in this report.

The current data report provides a simple representation and summary of the NTA results. Therefore, the description of methods and quality assurance are brief and high-level. Additional

[1] NJ DEP Report #3. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #1: Targeted Analysis of PFAS in Water Samples. U.S.EPA/ORD, April 17, 2019.

reports and/or publications are being developed that will include a more detailed description of methods, quality assurance analyses, and statistical/geospatial interpretation of the project data. As study partners/collaborators, we anticipate that NJ DEP and EPA Region 2 scientists will assist in these additional reports and publications.

Methods in Brief. Water samples were analyzed with high-performance liquid chromatography mass spectrometry (HPLC-MS) using methods described within our Quality Assurance Project Plan (QAPP)[2] and McCord et al. 2019.[3] In brief, water samples (500 mL) were filtered and then extracted using a WAX solid phase extraction cartridge. PFAS was removed from the cartridge in methanol and the methanol blown down to a volume of 1 mL under a gentle stream of dry nitrogen. An aliquot of the concentrated sample was injected into an Agilent high performance liquid chromatograph (HPLC) coupled to an Agilent time-of-flight mass spectrometer (TOFMS).

PFAS were analyzed using NTA methods. NTA provides two important measurements. The first is a tentative identification of PFAS compounds detected in the sample based on a combination of mass spectral data along with patterns of fragmentation compared to on-line and in-house mass-spectral libraries. Analytes in each sample and process blank were identified to various levels of confidence depending on the combined evidence from manual examination of MS/MS fragmentation spectra and/or comparison with mass spectral libraries.

The second type of information is an indication of the relative abundance of the PFAS present in the sample. The MS detector provides integrated peak areas for the chromatogram of the compound mass (+/- 5 ppm) at the specified retention time. The peak area is proportional to the mass of PFAS in the sample. Since the sample and injection volume are held constant, the peak area counts are also proportional to concentration, although the relationship varies based on compound.

It is important to understand how NTA results differ from those produced during routine laboratory targeted analysis. Without a standard curve to calibrate the relationship between peak area and a mass or concentration value, the peak area alone should be considered a semi-quantitative indicator of relative abundance. Analyte peak areas can be compared between samples in a sample set to obtain relative concentrations but cannot be directly compared between analytes. Our experience indicates that measured abundances for PFAS are four to six orders of magnitude higher than quantitated concentrations (e.g. 1e7 ~ 100 ppt). Peak area is expected to have much greater inherent sampling and analytical variability than standards-based analyses, which may become evident in reproducibility assessments. For example, it is possible for field duplicates to differ by two to three-fold or more, and laboratory replicates to have

[2] National Exposure Research Laboratory, Quality Assurance Project Plan: Detection, Evaluation and Assignment of Multiple Poly and Per-fluoroalkyl Substances (PFAS) in environmental media from an industrialized area of New Jersey. Prepared for New Jersey Department of Environmental Protection (NJ DEP), September 14, 2017.

[3] McCord, J., Strynar, M. Identifying Per- and Polyfluorinated Chemical Species with a Combined Targeted and Non-Targeted-Screening High-Resolution Mass Spectrometry Workflow. *J. Vis. Exp.* (146), e59142, doi:10.3791/59142 (2019). https://www.jove.com/video/59142/identifying-per-polyfluorinated-chemical-species-with-combined

greater variability than typically observed in routine laboratory analysis. Any application of NTA results should consider this inherently greater uncertainty.

The NTA data generated by HPLC-MS were considered as a "detect" when acceptable chromatographic peaks and spectra were evident. Samples without a detectable peak are reported as "ND" or not detected. Samples with detected analytes were further screened to determine the reporting limit (RL) that accounts for contamination that may have occurred during sampling and analysis, including field, laboratory, and instrument blanks. The RL was established for each compound by statistical analysis of the combined laboratory and field blanks according to Equation 1. Sample values less than this threshold are reported as "<RL".

Equation 1. Reporting Limit (RL) =Average [Field and Laboratory blanks] + 3x STD [blanks].

Summary of Results. All samples were analyzed with HPLC-MS methods as described above. Results are presented in 4 sections in this report as follow:

A. General NTA Abundance of PFAS Based on Peak Area for the 70 samples processed as a group,

B. Compound Identification and Peak Area for 3 Samples collected at FPPW001 and processed separately,

C. Additional Semi-Quantitation of Chloro-Perfluoro-Polyether- Carboxylate (ClPFPECA) in the samples presented in section A, and

D. QA/QC Discussion.

A. General NTA Abundance of PFAS Based on Peak Area

This section provides NTA results for 70 water samples and field blanks collected from tidal and non-tidal surface water and groundwater wells primarily from October 17 to December 11, 2017 and received at the ORD laboratory in Research Triangle Park during November and December 2017.

<u>Compound Identification:</u> Across all the water samples, we detected and tentatively identified 38 additional PFAS not previously quantitated in Report #3. These PFAS are listed in Table 2 by compound name, CAS registry number (CASRN; where available), chemical formula, monoisotopic mass, and retention time. A large number of chemical features likely to be PFAS (or breakdown products) were present, but we report these 38 compounds based on criteria of abundance (or peak area) relative to field and laboratory blanks and high confidence in tentative identification. Whereas tentative formulas are provided for all 38 PFAS, a CASRN is only available for 30 of the compounds. These same 30 PFAS are registered in EPA's CompTox

Chemicals Dashboard[4] where additional information about these chemicals can be found. NTA analysis of these water samples identified the presence of the congener series named Chloro-Perfluoro-Polyether- Carboxylate (ClPFPECA, Chem. Ref. #11 in Table 2) that were previously found in soils, vegetation, sediment and well water.

Abundance of Compounds: NTA results are provided as uncalibrated peak area abundances for the various water samples received in Tables 3-6. Samples are presented using the identifiers provided on the Chain of Custody forms received from NJ DEP. Note that naming conventions vary among samples and sample numbers are not always sequential.

Table 3 contains results for 30 well samples, including 25 samples and 5 duplicates collected from wells in November and December 2017 and labeled PFPW. One of these well samples and duplicate (PFPPW 002) were collected April 20, 2017 and one sample and duplicate labeled PFIND were received on December 7, 2017. Table 4 includes results for 11 samples and 2 duplicates collected from non-tidal surface water and labeled PFNSW. Table 5 includes results for 19 samples and 2 duplicates collected from tidal surface waters and labeled PFTSW. (Note that Table 5 does not provide results for sample PFTSW013 that was received but is not reported because the analyst did not have confidence in the analytical results.) Table 6 provides results for 6 field blanks (5 trip blanks and 1 field blank) and 8 laboratory blanks.

Color	Peak Area Category
ND	No peak area detected
<RL	Less than reporting limit
	>RL - 50,000
	50,000 - 100,000
	100,000 - 200,000
	200,000 - 500,000
	500,000 - 1,000,000
	>1,000,000

In Tables 3-6, the peak areas are superimposed on a heat map where gradations in color reflect seven classifications of peak area from low (non-detect and less than the reporting limit) to high (>1,000,000). The heat-map is useful in showing where PFAS "light-up" in terms of detection and high peak areas. The heat-map is intended to be a visual gradient for display purposes only. Heat map values >50,000 (yellow, orange, and red tones) have the highest confidence that a compound is present in relatively greater abundance. Note that relative abundances of the same analyte can be compared among samples (i.e., along rows in the results tables); however, because the results are neither normalized nor calibrated, peak areas should not be compared between compounds.

In processing samples, the sample volume injected into the HPLC-MS determines the peak area count. The samples included in Tables 3-6 were processed in two batches in which samples in one batch were injected with a volume of 40 µL whereas the samples in the other batch were injected with a volume of 5 µL. The reported sample results in Tables 3-6 were adjusted to a common reference by dividing peak areas of the samples injected at 40 µL by eight (8). Analytes that may have been present in samples at low concentrations may have been less likely to be

[4] U.S. EPA CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard

detected when injected at the 5 μL volume. The injection volume of each sample is shown in the bottom row of the tables.

Some of the identified compounds were widely distributed but detected in relatively low abundances (e.g., Chem. Ref. # 12). Conversely, some compounds were detected in elevated abundances in samples from only one location (e.g., PFNSW004, Table 4). The majority of sample/analyte results (88%) were non-detect (ND) or less than the reporting limit. The compound ClPFPECA (Chem. Ref. # 11) was observed in elevated abundances at multiple sampling locations.

Several blanks (Table 6) had detectable peak areas for many of the analytes but their peak area abundances were less than the reporting limit (<RL). One laboratory blank, DB7, was contaminated with measurable levels of several PFAS compounds.

Comparison of duplicates is the only method available for assessment of the reproducibility in the samples. There were 9 duplicate pairs. Within the combined group, duplicate pairs agreed that a sample was non-detect (ND), <RL, or less than a minimum 20,000 peak area in 92% of the comparisons. The Relative Percent Difference (RPD) of duplicate samples is used as an indicator of the repeatability of sampling calculated as follows:

Equation 2. Relative Percent Difference (RPD) = $ABS(X_1-X_2)/((X_1+X_2)/2)$

There were just 7 duplicate sample comparisons in which peak areas exceeded 20,000 in both samples allowing for the calculation of the RPD. The RPDs averaged 23% and were within project goals of ±50% applied to targeted analysis. It is evident in Tables 3-5 that multiple analytes in some duplicate pairs did not match well. Analytical reproducibility of these samples will be further explored in Section D.

Finally, we note that some of the groundwater wells were resampled in Sept 2019 with NTA results provided in NJ DEP Report #7[5]. NTA results for these same wells included in Table 3 of this report are not expected to be comparable to those results presented in Report #7 due to differences in methods, time lag, and analytical instruments used in the analyses. The samples in Table 3 were processed with a HPLC-TOFMS and minimal manual interpretation of spectral features. In contrast, sample results presented in Report #7 were analyzed on an UPLC-Orbitrap MS and processed with significant manual interpretation.

[5] NJDEP Report #7. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #7: Non-targeted Analysis of PFAS in Water Samples Collected from Wells with Point of Entry Treatment. U.S.EPA/ORD, April 23, 2020

Table 2. PFAS Tentatively Identified in Water Samples by HPLC-MS Non-targeted Analysis excluding PFAS previously quantified with standards in NJ DEP Report #3.

Chem. Ref. #	Tentatively Identified Compound Name	CAS Registry Number	Formula	Monoisotopic Mass (Daltons)	Retention Time
1	Perfluoropropanoic acid	422-64-0	C3 H F5 O2	163.9903	0.96
2	Perfluorododecanoic acid (PRDoDA)	307-55-1	C12 H F23 O2	613.9591	8.33
3	Perfluoropentanesulfonate (PFPeS)	2706-91-4	C5 H F11 O3 S	349.9471	5.61
4	Perfluoroheptanesulfonic acid (PFHpS)	375-92-8	C7 F15 H O3 S	449.9400	6.71
5	Perfluorononanesulfonic acid (PFNS)	68259-12-1	C9 H F19 O3 S	549.9322	7.48
6	2:2 fluorotelomer alcohol	54949-74-5	C4 H5 F5 O	164.0226	1.10
7	4:2 Fluorotelomer sulfonic acid (4:2FtS)	757124-72-4	C6 H5 F9 O3 S	327.9826	5.36
8	6:2 Fluorotelomer sulfonic acid (6:2FtS)	27619-97-2	C8 H5 F13 O3 S	427.9751	6.64
9	7:2 Fluorotelomer dihydrogen phosphate	37013-72-2	C9 H6 F15 O4 P	493.9763	7.36
10	8:2 Fluorotelomer sulfonic acid (8:2FtS)	39108-34-4	C10 H5 F17 O3 S	527.9677	7.47
11	ClPFPECA 0,1 (Chloro-Perfluoro=Polyether-Carboxylate) fragment	-	C8 CL F14 O4	367.9480	7.02
12	N,N-dimethyl-2H-perfluoroethanamine	1550-50-1	C4 H7 F4 N	145.0540	3.14
13	1,1,1,2-Tetrafluoro-3,3,3-trimethoxypropane	42415-18-9	C6 H10 F4 O3	206.0563	1.33
14	2-Perfluoropropyl-2-propanol	355-22-6	C6 H7 F7 O	227.0427	2.25
15	5H-Perfluoropentanal	2648-47-7	C5 H2 F8 O	229.9938	1.05
16	Ethyl 4,4,4-trifluoro-3-(trifluoromethyl)crotonate	1513-60-6	C7 H6 F6 O2	236.0350	0.70
17	1,4-Bis(1,1-dimethylethyl)-2,3,5,6-tetrafluorobenzene	54111-17-0	C14 H18 F4	262.1400	4.58
18	1H,1H,5H,5H-Perfluoro-1,5-pentanediol diacrylate	678-95-5	C11 H10 F6 O4	320.0495	1.34
19	Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis-, dipotassium salt	-	C15 H10 F6 O2	336.0603	4.90
20	((Perfluorobutyl)ethyl)trimethoxysilane	85877-79-8	C9 H13 F9 O3 Si	368.0558	0.58
21	1-Hydroperfluoroheptane	61915-92-2	C12 H12 F10 O2	378.0761	0.67
22	3,3,4,4,5,5,6,6,7,7-Decafluorooctyl 2-methylprop-2-enoate	139702-34-4	C7 H F13 O3	379.9721	6.33
23	Tridecafluoroheptaneperoxoic acid	-	C8 H12 F9 N O4 S	389.0297	6.37
24	C8H12F9NO4S	68555-78-2	C10 H13 F11 N2 O2 S	434.0591	4.22
25	Perfluoropentane sulfonamido amine	57678-01-0	C8 H6 F13 O4 P	443.9812	6.98
26	6:2 Fluorotelomer phosphate monoester	-	C14 H17 F13 O	448.1024	4.06
27	C14H17F13O	-	C11 H6 Cl F13 O2	451.9865	6.77
28	C11H6ClF13O2	-	C9 H3 F17 O3	481.9771	7.15
29	C9H3F17O3	754-91-6	C8 H2 F17 N O2 S	498.9501	6.70
30	Perfluorooctanesulfonamide (PFOSA)	1765-48-6	C11 H2 F20 O2	545.9735	7.15
31	11-H-Perfluoroundecanoic acid	230295-05-3	C13 H5 F17 O4	547.9887	7.71
32	Monoperfluorooctyl itaconate	68957-57-3	C11 H16 F11 I N2 O2 S	575.9825	7.04
33	POLYFLGSID_880938	203302-98-1	C12 H3 F21 O2	577.9789	7.29
34	Methyl perfluoroundecanoate	-	C10 H F21 O3 S	599.9310	7.85
35	Henicosafluorodecanesulphonate	-	C13 H F25 O2	663.9548	9.13
36	Dodecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,12,12,12-docosafluoro-11-(trifluoromethyl)-, compd. with ethanamine (1:1)	72494-14-5	C33 H42 F8 N2 O4	682.3009	13.30
37	POLYFLGSID_880958	32687-76-6	C14 H2 F24 O4	689.9555	6.38
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoyl) peroxide	37486-69-4	C17 H F35 O5	949.9221	7.00

Table 3. PFAS Peak Area for Groundwater Wells Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFIND 026	PFIND 026 DUP	PFPPW 002	PFPPW 002 DUP	PFPW 002	PFPW 003	PFPW 004	PFPW 005	PFPW 007	PFPW 008	DUP
1	Perfluoropropanoic acid	<RL	<RL	<RL	<RL	ND	<RL	ND	<RL	ND	ND	94,800
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	2,660	ND	2,170	2,700	ND	ND	ND	ND	ND	ND	ND
4	PFHpS	1,060	ND	1,160	1,750	ND	ND	ND	ND	ND	ND	ND
5	PFNS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	3,310	ND	<RL	<RL	ND	39,300	ND	166,000	4,560	ND	4,010
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	ND	<RL	<RL	<RL	ND	ND	ND	ND	ND	ND	ND
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	<RL	<RL	<RL	<RL	<RL	214,000	<RL	<RL	431,000	ND	2,240,000
12	N,N-dimethyl-2H- . . .	25,500	27,700	1,190	1,650	ND	27,800	15,500	232,000	44,700	ND	21,200
13	1,1,1,2-Tetrafluoro . . .	23,600	ND	20,300	14,200	ND	ND	ND	<RL	ND	ND	ND
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND	ND	8,190	ND	ND	11,700	ND	13,500
15	5H-Perfluoropentanal	<RL	ND	ND	ND	174,000	373,000	359,000	284,000	254,000	252,000	360,000
16	Ethyl 4,4,4-trifluoro-3 . . .	51,600	30,800	<RL	<RL	36,200	<RL	41,200	32,100	<RL	ND	34,700
17	1,4-Bis(1,1-dimethylethyl)-. . .	10,100	ND	6,370	5,700	ND	ND	ND	ND	ND	ND	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	<RL	ND	<RL	ND	26,500	23,400	26,500	18,500	23,600	ND	25,600
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	17,800	ND	ND	ND	ND	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	ND	8,900	ND	ND	<RL	ND	ND	6,330	7,310	ND	8,330
21	1-Hydroperfluoroheptane	ND	17,200	<RL	<RL	14,000	<RL	18,000	ND	<RL	ND	7,590
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	6,930	<RL	<RL	ND	ND	ND	ND	ND	ND	ND
23	Tridecafluoroheptaneperoxoic acid	7,730	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	2,100	ND	ND	ND	ND	ND	10,200	ND	ND	ND	ND
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
28	C11H6ClF13O2	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
29	C9H3F17O3	12,400	ND	ND	<RL	ND	ND	ND	ND	ND	ND	ND
30	PFOSA	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	ND	<RL	<RL	ND	<RL	<RL	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	13,100	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***40***	***5***	***40***	***40***	***5***	***5***	***5***	***5***	***5***	***5***	***5***

Table 3. (Continued) PFAS Peak Area for Groundwater Wells Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFPW 009	PFPW 010	PFPW DUP2	PFPW 011	PFPW 012	PFPW DUP1	PFPW 013D	PFPW 013I	PFPW 013S
1	Perfluoropropanoic acid	ND	ND	<RL	ND	<RL	ND	<RL	<RL	<RL
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	ND	ND	ND	ND	ND	ND	ND	ND	ND
4	PFHpS	ND	ND	ND	ND	ND	ND	ND	ND	ND
5	PFNS	ND	ND	ND	14,600	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	5,360	ND	ND	ND	5,180	ND	ND	ND	ND
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	<RL	<RL	<RL	ND	<RL	ND	<RL	22,900	ND
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	4,140,000	2,800,000	3,050,000	1,030,000	633,000	ND	3,520,000	4,520,000	<RL
12	N,N-dimethyl-2H- . . .	29,300	32,900	19,800	17,300	36,200	ND	22,800	27,600	ND
13	1,1,1,2-Tetrafluoro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
14	2-Perfluoropropyl-2-propanol	24,700	24,300	30,500	36,700	15,800	ND	23,200	19,700	ND
15	5H-Perfluoropentanal	<RL	ND	ND	ND	<RL	ND	ND	ND	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL	31,900
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	14,900	15,400	ND	15,300	11,800	ND	<RL	ND	8,600
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	ND	<RL	6,220	6,040	<RL	ND	ND	ND	ND
21	1-Hydroperfluoroheptane	ND	ND	ND	10,900	6,880	ND	<RL	<RL	19,500
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	ND	6,710	ND	ND	ND	ND	ND	ND
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	ND	ND	ND	ND	ND	ND	ND	ND	ND
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	<RL	ND	<RL	<RL	<RL	ND	<RL	<RL
28	C11H6ClF13O2	ND	<RL	ND	<RL	ND	<RL	<RL	ND	<RL
29	C9H3F17O3	ND	ND	ND	ND	ND	ND	ND	ND	ND
30	PFOSA	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	ND	<RL	<RL	<RL	<RL	<RL	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***

Table 3. (Continued) PFAS Peak Area for Groundwater Wells Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFPW 014	PFPW 015	PFPW 016	PFPW 017	PFPW 019	PFPW 020	PFPW 021	PFPW 022	PFPW 024	PFPW 025
1	Perfluoropropanoic acid	ND	<RL	<RL	ND	<RL	<RL	ND	ND	ND	ND
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	ND	ND	ND	ND	ND	5,810	47,400	275,000	39,200	ND
4	PFHpS	ND	ND	ND	ND	ND	ND	49,700	268,000	38,600	ND
5	PFNS	ND	ND	ND	ND	ND	ND	17,000	68,000	13,000	ND
6	2:2 fluorotelomer alcohol	19,100	ND	ND	10,000	8,080	ND	ND	ND	ND	ND
7	4:2 FtS	ND	ND	ND	ND	ND	ND	7,620	39,000	6,650	ND
8	6:2 FtS	ND	ND	ND	ND	ND	ND	<RL	40,000	<RL	ND
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	12,800	ND	ND
11	ClPFPECA 0,1 fragment	467,000	<RL	780,000	881,000	676,000	<RL	ND	ND	ND	ND
12	N,N-dimethyl-2H- . . .	87,000	19,900	15,400	20,300	23,200	ND	ND	ND	ND	ND
13	1,1,1,2-Tetrafluoro . . .	<RL	ND	ND	12,400	ND	ND	ND	ND	ND	ND
14	2-Perfluoropropyl-2-propanol	ND	ND	15,300	11,400	16,200	ND	ND	ND	ND	ND
15	5H-Perfluoropentanal	<RL	ND	<RL	ND	127,000	<RL	ND	ND	ND	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	<RL	<RL	<RL	<RL	31,900	ND	ND	ND	ND	ND
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	ND	ND	<RL	ND	6,330	ND	ND	ND	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	11,900	10,100	8,020	15,100	9,470	10,800	ND	ND	ND	ND
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	10,500	4,990	<RL	<RL	<RL	ND	ND	ND	ND	ND
21	1-Hydroperfluoroheptane	<RL	6,680	8,470	ND	12,300	ND	ND	ND	ND	ND
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	5,360	10,500	ND	ND	ND	ND	ND	ND	ND	ND
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL	<RL
28	C11H6ClF13O2	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL	ND	<RL
29	C9H3F17O3	ND	ND	ND	ND	ND	ND	ND	10,700	ND	ND
30	PFOSA	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	5,790	22,800	5,130	ND
35	Henicosafluorodecanesulphonate	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***

Table 4. PFAS Peak Area for Non-tidal Surface Water Samples Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFNSW 003	PFNSW 004	PFNSW DUP2	PFNSW 005	PFNSW 012	PFNSW 014	PFNSW 017	PFNSW 018	PFNSW DUP1
1	Perfluoropropanoic acid	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
2	PRDoDA	ND	56,600	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	3,080	ND	618	ND	807	ND	ND	30,900	36,900
4	PFHpS	1,560	ND	ND	ND	694	ND	ND	7,260	10,200
5	PFNS	ND	ND	ND	ND	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	5,580	ND	ND	ND	44,600	ND	ND	12,500	15,100
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	<RL	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL
9	7:2 Fluorotelomer dihydro . . .	ND	14,500	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
12	N,N-dimethyl-2H- . . .	60,500	12,100	10,700	10,500	25,700	5,110	16,600	57,700	69,200
13	1,1,1,2-Tetrafluoro . . .	14,900	12,600	11,900	14,900	11,700	9,260	20,000	10,300	24,600
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND	ND	ND	ND	ND	596
15	5H-Perfluoropentanal	ND	<RL	ND	<RL	<RL	ND	<RL	ND	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
17	1,4-Bis(1,1-dimethylethyl)-. . .	<RL	ND	ND	ND	ND	ND	ND	ND	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	<RL	<RL	ND	<RL	<RL	ND	ND	<RL	ND
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	546	ND	ND	ND	3,130	ND	ND	16,400	15,100
20	((Perfluorobutyl)ethyl) . . .	<RL	ND	5,170	<RL	<RL	<RL	7,630	<RL	5,000
21	1-Hydroperfluoroheptane	ND	7,720	ND	ND	ND	<RL	ND	ND	5,850
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	1,990	ND	ND	132,000	ND	ND	ND	<RL
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	3,970	4,320	11,000	6,700	4,200	9,380	ND	ND	487
25	Perfluoropentane . . .	ND	20,500	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	795	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	98,300	<RL	<RL	<RL	<RL	<RL	<RL	<RL
28	C11H6ClF13O2	<RL	96,200	<RL	<RL	<RL	<RL	<RL	<RL	<RL
29	C9H3F17O3	ND	ND	ND	ND	ND	ND	ND	ND	ND
30	PFOSA	<RL	694,000	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	6,880	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	4,270	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	22,200	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	<RL	3,900,000	ND	ND	ND	ND	ND	ND	ND
36	Dodecanoic acid . . .	<RL	758,000	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	227,000	<RL	<RL	<RL	<RL	<RL	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***40***	***40***	***40***	***40***	***40***	***40***	***40***	***40***	***40***

Table 4. (Continued) PFAS Peak Area for Non-tidal Surface Water Samples Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFNSW 019	PFNSW 020	PFNSW 023	PFNSW 025
1	Perfluoropropanoic acid	<RL	<RL	<RL	<RL
2	PRDoDA	ND	ND	ND	ND
3	PFPeS	ND	ND	1,330	1,080
4	PFHpS	744	ND	961	ND
5	PFNS	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	ND	<RL	ND	<RL
7	4:2 FtS	ND	ND	ND	ND
8	6:2 FtS	<RL	ND	ND	<RL
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	<RL	<RL	<RL	<RL
12	N,N-dimethyl-2H- . . .	11,900	20,300	20,300	16,200
13	1,1,1,2-Tetrafluoro . . .	16,700	<RL	11,700	11,200
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND
15	5H-Perfluoropentanal	ND	ND	ND	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	<RL	<RL	<RL	<RL
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	<RL	ND	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	ND	ND	ND	ND
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	12,800	968	ND
20	((Perfluorobutyl)ethyl) . . .	<RL	ND	<RL	6,210
21	1-Hydroperfluoroheptane	31,600	ND	ND	ND
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	<RL	ND	ND	<RL
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND
24	C8H12F9NO4S	ND	427	13,800	2,810
25	Perfluoropentane . . .	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	30,200	ND	7,860	ND
27	C14H17F13O	<RL	<RL	<RL	<RL
28	C11H6ClF13O2	<RL	<RL	<RL	<RL
29	C9H3F17O3	<RL	ND	ND	ND
30	PFOSA	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	ND	ND	ND	ND
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	<RL	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND
	Injection Volume (µL)	***40***	***40***	***40***	***40***

Table 5. PFAS Peak Area for Tidal Surface Water Samples Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFTSW 001	PFTSW 002	PFTSW 003	PFTSW 004	PFTSW 005	PFTSW 006	PFTSW 007	PFTSW 008	PFTSW 009	PFTSW 010	PFTSW DUP2
1	Perfluoropropanoic acid	<RL	ND	ND	<RL	<RL	<RL	<RL	ND	<RL	<RL	<RL
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	1,300
4	PFHpS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	625
5	PFNS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	5,880
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	<RL
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	CIPFPECA 0,1 fragment	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	1,950,000
12	N,N-dimethyl-2H- . . .	ND	ND	21,100	ND	9,440	ND	ND	ND	ND	ND	27,900
13	1,1,1,2-Tetrafluoro . . .	ND	ND	ND	<RL	ND	9,930	ND	ND	6,920	ND	13,300
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	16,500
15	5H-Perfluoropentanal	ND	ND	ND	ND	ND	ND	ND	ND	ND	<RL	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	ND	<RL	ND	31,100	ND	<RL	<RL	<RL	ND	ND	<RL
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	5,710	ND	ND	6,130	ND	ND	ND	7,610	ND	<RL
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	ND	ND	ND	<RL	ND	<RL	ND	ND	ND	ND	<RL
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	ND	ND	ND	5,170	ND	<RL	ND	ND	ND	ND	<RL
21	1-Hydroperfluoroheptane	ND	<RL	ND	21,900	ND	8,220	ND	<RL	5,840	ND	<RL
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	1,780
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	<RL	<RL	ND	<RL	ND	<RL	ND	<RL	ND	<RL
28	C11H6ClF13O2	<RL	<RL	ND	<RL	<RL	ND	<RL	<RL	ND	<RL	ND
29	C9H3F17O3	ND	ND	ND	ND	ND	7,530	ND	ND	ND	ND	ND
30	PFOSA	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	<RL	ND	ND	<RL	<RL	<RL	ND	ND	<RL	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***40***

Table 5. (Continued) PFAS Peak Area for Tidal Surface Water Samples Determined with Non-targeted Analysis.

Chem. Ref. #	Compound	PFTSW 011	PFTSW 012	PFTSW 014	PFTSW 015	PFTSW DUP1	PFTSW 016	PFTSW 017	PFTSW 018	PFTSW 019	PFTSW 020
1	Perfluoropropanoic acid	<RL	<RL	ND	<RL	<RL	<RL	59,800	57,500	<RL	<RL
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	ND	ND	ND	ND	919	ND	10,800	ND	ND	ND
4	PFHpS	ND	ND	ND	ND	598	ND	18,800	ND	ND	4,670
5	PFNS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	ND	ND	ND	ND	4,490	ND	2,360	ND	ND	ND
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	<RL	ND	ND	ND	<RL	ND	<RL	ND	ND	ND
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	<RL	ND	ND	<RL	1,530,000	ND	ND	ND	ND	ND
12	N,N-dimethyl-2H- . . .	ND	ND	ND	ND	27,200	ND	ND	ND	ND	ND
13	1,1,1,2-Tetrafluoro . . .	ND	6,880	ND	<RL	16,800	ND	ND	<RL	ND	6,690
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND	11,500	ND	ND	ND	ND	ND
15	5H-Perfluoropentanal	ND	ND	ND	ND	<RL	ND	ND	<RL	ND	ND
16	Ethyl 4,4,4-trifluoro-3 . . .	<RL	<RL	ND	37,300	<RL	ND	35,500	<RL	<RL	<RL
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	<RL	ND	ND	<RL	ND	ND	<RL	ND	9,050
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	<RL	ND	ND	ND	<RL	ND	ND	<RL	ND	ND
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	ND	ND	ND	577	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	ND	ND	ND	<RL	<RL	ND	ND	ND	ND	ND
21	1-Hydroperfluoroheptane	18,600	<RL	ND	<RL	<RL	ND	31,400	<RL	ND	ND
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	ND	ND	ND	ND	1,160	ND	ND	ND	ND	ND
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	<RL	ND	ND	<RL	<RL	ND	<RL	ND	ND	ND
28	C11H6ClF13O2	ND	ND	ND	ND	<RL	ND	<RL	ND	ND	ND
29	C9H3F17O3	ND	6,710	16,100	<RL	ND	ND	ND	ND	ND	10,400
30	PFOSA	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	<RL	ND	ND	ND	<RL	ND	<RL	<RL	ND	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***5***	***5***	***5***	***5***	***40***	***5***	***5***	***5***	***5***	***5***

Table 6. PFAS Peak Area for Laboratory and Field Blanks Determined with Non-targeted Analysis.

		Laboratory Blanks								Field Blanks					
Chem. Ref. #	Compound	DB1	DB2	DB3	DB4	DB5	DB6	DB7	DB8	PFNSW TB	PFPW TB1	PFPW TB2	PFTSW FB1	PFTSW TB1	PFTSW TB2
1	Perfluoropropanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	<RL	<RL	ND	<RL	ND
2	PRDoDA	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
3	PFPeS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
4	PFHpS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
5	PFNS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
6	2:2 fluorotelomer alcohol	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	2,460	ND	ND	ND
7	4:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
8	6:2 FtS	ND	ND	ND	ND	ND	ND	18,400	ND	ND	ND	ND	ND	ND	ND
9	7:2 Fluorotelomer dihydro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	8:2 FtS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
11	ClPFPECA 0,1 fragment	ND	<RL	<RL	<RL	<RL	<RL	<RL	<RL	ND	ND	ND	<RL	<RL	<RL
12	N,N-dimethyl-2H- . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
13	1,1,1,2-Tetrafluoro . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	7,640	ND	ND
14	2-Perfluoropropyl-2-propanol	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
15	5H-Perfluoropentanal	ND	<RL	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	<RL	115,000
16	Ethyl 4,4,4-trifluoro-3 . . .	ND	<RL	<RL	<RL	<RL	<RL	<RL	<RL	ND	<RL	ND	ND	<RL	ND
17	1,4-Bis(1,1-dimethylethyl)-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	6,420	ND
18	1H,1H,5H,5H-Perfluoro-1,5-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	7,440	ND	<RL	ND	ND
19	Phenol, 4,4'-[2,2,2-trifluoro-. . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
20	((Perfluorobutyl)ethyl) . . .	ND	ND	ND	ND	<RL	<RL	ND	<RL	ND	ND	ND	ND	ND	ND
21	1-Hydroperfluoroheptane	ND	ND	ND	<RL	ND	ND	5,640	ND	ND	ND	ND	ND	ND	ND
22	3,3,4,4,5,5,6,6,7,7-Decafluoro. . .	ND	ND	ND	ND	ND	ND	ND	ND	<RL	ND	ND	ND	ND	<RL
23	Tridecafluoroheptaneperoxoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
24	C8H12F9NO4S	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
25	Perfluoropentane . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26	6:2 Fluorotelomer phosphate . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27	C14H17F13O	ND	ND	ND	<RL	ND	<RL	66,800	<RL	<RL	<RL	ND	<RL	ND	<RL
28	C11H6ClF13O2	ND	ND	<RL	ND	ND	<RL	89,500	<RL	<RL	ND	ND	<RL	ND	<RL
29	C9H3F17O3	ND	ND	ND	ND	ND	ND	ND	ND	ND	6,950	ND	ND	ND	ND
30	PFOSA	ND	<RL	<RL	<RL	<RL	<RL	494,000	<RL	<RL	<RL	<RL	<RL	<RL	<RL
31	11-H-Perfluoroundecanoic acid	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
32	Monoperfluorooctyl itaconate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33	POLYFLGSID_880938	ND	ND	ND	ND	ND	ND	16,200	ND	ND	ND	ND	ND	ND	ND
34	Methyl perfluoroundecanoate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
35	Henicosafluorodecanesulphonate	ND	<RL	<RL	<RL	<RL	<RL	<RL	<RL	ND	<RL	<RL	<RL	<RL	<RL
36	Dodecanoic acid . . .	ND	<RL	<RL	<RL	<RL	<RL	181,000	<RL	<RL	<RL	<RL	<RL	<RL	<RL
37	POLYFLGSID_880958	ND	<RL	<RL	ND	ND	<RL	144,000	<RL	<RL	<RL	<RL	<RL	ND	<RL
38	Bis(2,2,3,3,4,4,5,5,6,6,7,7 . . .	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Injection Volume (µL)	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***5***	***40***	***5***	***5***	***40***	***40***	***40***

B. Compound Identification and Peak Area for Samples collected at FPPW001

This section provides NTA results for 2 water samples, 1 field blank collected at a well FPPW 001 in August 2016, and 1 laboratory blank. Samples were prepared and analyzed with the same HPLC-MS methodology described for the samples reported in Section A. Targeted analysis results for 10 PFAS compounds were previously provided for these samples in NJ DEP Report #3[1].

Compound Identification: We detected and tentatively identified 12 PFAS in samples collected at FPPW 001 that were not previously quantitated in Report #3. These compounds are listed by compound name, CAS registry number (CASRN), chemical formula, and monoisotopic mass in Table 7. A large number of chemical features likely to be PFAS (or breakdown products) were present, but we report these 12 based on criteria of abundance (or peak area) relative to field and laboratory blanks, and high confidence in tentative identification. These 12 PFAS are registered in EPA's CompTox Chemicals Dashboard[4] where additional information about these chemicals can be found.

Three of the PFAS compounds listed in Table 7 were identified at FPPW 001 were also found in some of the samples presented in Tables 3-5 (Chem. Ref. #'s 1, 16, and 29). Nine additional analytes listed in Table 7 were uniquely identified in the samples from FPPW 001 (Chem. Ref. #'s 39-47). Table 7 appends chemical reference #s to those in Table 2. NTA analysis did not identify the presence of the ClPFPECA congener series in the FPPW 001 samples (Chem. Ref. #11 in Table 2). With the additional analytes observed at this well location, a total of 47 different PFAS analytes were found in these water samples in addition to the 10 PFAS previously quantitated in NJ DEP Report #3[1].

Table 7. PFAS Tentatively Identified in Water Samples at FPPW 001 by HPLC-MS Non-targeted Analysis excluding PFAS previously quantified with standards in NJ DEP Report #3.

Chem. Ref. #	Tentatively Identified Compound Name	CAS Registry Number	Formula	Monoisotopic Mass (Daltons)
1	Perfluoropropanoic acid	422-64-0	C3 H F5 O2	163.99
16	Ethyl 4,4,4-trifluoro-3-(trifluoromethyl)crotonate	1513-60-6	C7 H6 F6 O2	236.03
29	Perfluorooctanesulfonamide	754-91-6	C8 H2 F17 N O2 S	498.95
39	ethyl 2,3,3,3-tetrafluoropropanoate	399-92-8	C5 H6 F4 O2	174.03
40	1H,2H-Hexafluorocyclopentene	1005-73-8	C5 H2 F6	176.01
41	3:2 Fluorotelomer alcohol	755-40-8	C5 H5 F7 O	214.02
42	2,2,3,3,4,4-Hexafluorobutyl 2-methylprop-2-enoate	45168-50-1	C8 H8 F6 O2	250.05
43	N-Methyl-N-trimethylsilylheptafluorobutyramide	53296-64-3	C8 H12 F7 N O Si	299.06
44	2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoyl Fluoride	5927-65-1	C7 H F13 O	347.98
45	Ammonium 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoate	376-34-1	C7 H5 F12 N O2	363.01
46	Undecafluorocyclohexanemethanol dihydrogen phosphate	32582-74-4	C7 H4 F11 O4 P	391.97
47	2H-Tricosafluoro-5,8,11,14-tetrakis(trifluoromethyl)-3,6,9,12,15-pentaoxaoctadecane	37486-69-4	C17 H F35 O5	949.92

Abundance of Compounds: Compound identification and NTA results for the unknown sample, a duplicate and a field blank collected at location FPPW 001 are provided as uncalibrated peak areas in Table 8. PFAS compounds whose concentrations were previously reported using targeted analysis in NJ DEP Report #3 were also detected with NTA but their peak areas are not reported here.

No analytes were detected in field or laboratory blanks. Repeatability among the duplicate pairs the RPDs averaged 22.3% with 11 of 12 individual analytes meeting project goals of ±50% applied to targeted analysis precision.

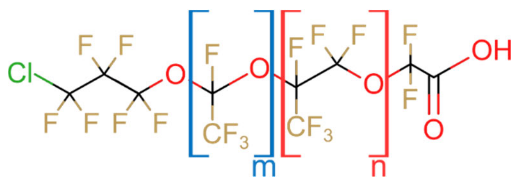
Table 8. PFAS Compounds and Peak Area for Samples Collected at FPPW 001 Determined with Non-targeted Analysis.

Chem. Ref. #	Tentatively Identified Compound	FPPW 001	FPPW 001Dup	Field Blank (BB)	Laboratory Blank (DB)
1	Perfluoropropanoic acid	58,600	65,200	ND	ND
16	Ethyl 4,4,4-trifluoro-3-(trifluoromethyl)crotonate	43,900	63,900	ND	ND
29	Perfluorooctanesulfonamide	256,000	266,000	ND	ND
39	ethyl 2,3,3,3-tetrafluoropropanoate	47,500	57,000	ND	ND
40	1H,2H-Hexafluorocyclopentene	48,800	58,500	ND	ND
41	3:2 Fluorotelomer alcohol	50,200	40,500	ND	ND
42	2,2,3,3,4,4-Hexafluorobutyl 2-methylprop-2-enoate	421,000	487,000	ND	ND
43	N-Methyl-N-trimethylsilylheptafluorobutyramide	29,700	26,000	ND	ND
44	2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoyl Fluoride	54,600	34,700	ND	ND
45	Ammonium 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoate	6,360	15,300	ND	ND
46	Undecafluorocyclohexanemethanol dihydrogen phosphate	44,200	44,400	ND	ND
47	2H-Tricosafluoro-5,8,11,14-tetrakis(trifluoromethyl)-3,6,9,12,15-pentaoxaoctadecane	55,700	54,100	ND	ND

C. Semi-Quantitation of Chloro-Perfluoro-Polyether-Carboxylate (ClPFPECA)

NTA analysis of the water samples listed in Tables 3-6 detected the presence of the congener series named Chloro-Perfluoro-Polyether-Carboxylate (ClPFPECA, Chem. Ref. #11 in Table 2) in many of the samples. Various members of this congener series were previously found in soils and vegetation[6], sediment[7], and well water[8]. The generic structure of the ClPFPECA congeners is shown in Figure 1.

Figure 1. Generic Structure of Chloro-Perfluoro-Polyether-Carboxylate (ClPFPECA).



As a result of the particular interest in the ClPFPECA congeners[9], a second analysis of the water samples to provide an additional semi-quantitative estimate of ClPFPECA concentration (ng/L) was performed. Analysis of soils[6] identified nine congeners with m and n varying from 0 to 3. This analysis of water samples identified five of the shorter chain ClPFPECA congeners with m and n values varying from 0 to 2. Table 9 provides the formula, and molecular mass for the 5 congeners found in water samples.

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[6] NJ DEP Report #2. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #2: Non-targeted Analysis of PFAS in Soil and Vegetation. U.S.EPA/ORD, March 8, 2019.

[7] NJ DEP Report #5. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #5: Non-targeted Analysis of PFAS in Sediment. U.S.EPA/ORD, April 23, 2020.

[8] NJ DEP Report #7. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #7: Non-targeted Analysis of PFAS in Water Samples Collected from Wells with Point of Entry Treatment. U.S.EPA/ORD, April 23, 2020

[9] Washington, et al., 2020 Science DOI: 10.1126/science.aba7127

Table 9. Characteristic LC/MS/MS analytical parameters of Chloro-Perfluoro-Polyether-Carboxylate (ClPFPECA) Congeners Identified in Water Using Non-Targeted Analysis.

	Chloro-perfluoro-polyether-carboxylate (ClPFPECA) congeners by group number of ethyl, propyl				
Ethyl, Propyl Groups	**1,0**	**0,1**	**2,0**	**1,1**	**0,2**
Anion Formula	$C_7ClF_{12}O_4$	$C_8ClF_{14}O_4$	$C_9ClF_{16}O_5$	$C_{10}ClF_{18}O_5$	$C_{11}ClF_{20}O_5$
Molecular Mass (Daltons)	**411.9371**	**461.934**	**527.9257**	**577.9225**	**627.9193**

Since there are no standards for ClPFPECA congeners, an estimate of their concentration is derived from the MS response for two stable isotope-labeled compounds ($^{13}C_4$-labeled perfluorooctane sulfonate ($^{13}C_4$-PFOS) and $^{13}C_4$-labeled perfluorooctanoic acid ($^{13}C_4$-PFOA) of known concentration to serve as an internal standard (IS). The concentration of ClPFPECA was estimated proportional to its peak area assuming the same instrument response as the labeled PFAS using Equation 3. Our experience with PFAS suggests that this means of estimation is within an order of magnitude of the actual concentration.

Equation 3. $$ClPFPECA_{Conc} = \frac{\text{ClPFPECA}_{PA} \times C^{13}PFOS\_OA_{Conc}}{C^{13}PFOS\_OA_{PA}}$$

Where:

$ClPFPECA_{Conc}$ is the semi-quantified ClPFPECA concentration (ng/L)

$ClPFPECA_{PA}$ is the ClPFPECA peak area

C^{13}-$PFOS\_OA_{Conc}$ is the known concentration of labeled PFOS (or PFOA) after spiking into the sample (ng/L)

C^{13}-$PFOS\_OA_{PA}$ is the peak area of the labeled PFOS or PFOA.

Table 10 provides the peak areas of the five ClPFPECA congeners, their sum, and the estimated concentration of the 0,1 (ethyl, propyl) congener expressed as PFOA IS-based and PFOS IS-based concentration (ng/L).

Of the five ClPFPECA congeners (carbon lengths 7-11), most of the peak area or mass was attributed to the 0,1 (ethyl, propyl) congener (C8), which comprised 63 to 100 percent of the total in 45 individual samples in which ClPFPECA was detected. The 0,1 congener also made up the majority of the mass in previous analyses of soil and vegetation and sediment samples analyzed for NJ DEP and presented in NJ DEP Report #3[6].

Table 10. Semi-Quantitation of Chloro-Perfluoro-Polyether-Carboxylate Congeners (ClPFPECA) in Water Samples. Concentration Values (ng/L) are Estimated Based on Labeled PFOA and PFOS.

	Fully Integrated Peak Area of ClPFPECA Congeners Identified by Ethyl, Propyl Group						Estimated Concentration of ClPFPECA 0,1 (by simple ratios to matrix internal standard in ng/L)		
Sample ID	1,0	0,1	2,0	1,1	0,2	Sum of Congeners	$^{13}C_4$-PFOA IS based	$^{13}C_4$-PFOS IS based	Average
PFIND 026	ND	54,800	ND	ND	ND	54,800	56	48	52
PFIND026 DUP	ND	31,200	ND	ND	947	32,147	30	30	30
PFPPW 002	118	950	ND	ND	ND	1,068	1	1	1
PFPPW 002DUP	ND	7,110	ND	ND	56	7,166	4	3	3
PFPW 002	ND	116,000	ND	ND	ND	116,000	98	43	71
PFPW 003	ND	203,000	ND	ND	ND	203,000	197	121	159
PFPW 004	ND	21,200	ND	ND	586	21,786	15	7	11
PFPW 005	ND	8,890	ND	ND	ND	8,890	8	5	7
PFPW 007	ND	415,000	1,250	ND	ND	416,250	317	164	241
PFPW 008	ND	2,280	ND	ND	ND	2,280	2	2	2
DUP	2,580	2,220,000	701	ND	622	2,223,903	2,060	1,070	1,570
PFPW 009	11,900	4,080,000	4,360	4,000	2,010	4,102,270	3,590	2,060	2,820
PFPW 010	3,120	2,770,000	1,970	4,860	833	2,780,783	2,430	1,710	2,070
PFPW DUP2	6,020	3,020,000	4,130	992	2,010	3,033,152	2,270	1,520	1,890
PFPW 011	1,020	1,020,000	594	1,230	1,080	1,023,924	662	485	574
PFPW 012	ND	620,000	817	ND	ND	620,817	485	280	383
PFPW DUP1	615	ND	ND	ND	ND	615	-	-	-
PFPW 013D	8,720	3,480,000	2,700	998	3,280	3,495,698	2,510	1,690	2,100
PFPW 013i	13,700	4,450,000	8,600	2,820	3,400	4,478,520	3,740	2,210	2,970
PFPW 013S	ND	11,900	ND	ND	ND	11,900	9	5	7
PFPW 014	1,110	461,000	ND	ND	ND	462,110	359	273	316
PFPW 015	ND	33,200	ND	ND	ND	33,200	26	16	21
PFPW 016	ND	765,000	ND	ND	ND	765,000	664	451	558
PFPW 017	638	859,000	ND	679	589	860,906	568	341	454
PFPW 019	ND	664,000	790	681	1,420	666,891	460	277	368
PFPW 020	ND	33,300	ND	ND	ND	33,300	23	15	19
PFPW 021	ND	985	ND	ND	ND	985	1	1	1
PFPW 022	750	1,440	ND	ND	ND	2,190	1	1	1
PFPW 024	ND	ND	ND	ND	ND	0	-	-	-
PFPW 025	ND	ND	ND	ND	ND	0	-	-	-

Table 10. (Continued). Semi-Quantitation of Chloro-Perfluoro-Polyether-Carboxylate Congeners (ClPFPECA) in Water Samples. Concentration Values (ng/L) are Estimated Based on Labeled PFOA and PFOS.

	Fully Integrated Peak Area of ClPFPECA Congeners Identified by Ethyl, Propyl Group						Estimated Concentration of ClPFPECA 0,1 (by simple ratios to matrix internal standard in ng/L)		
Sample ID	1,0	0,1	2,0	1,1	0,2	Sum of Congeners	$^{13}C_4$-PFOA IS based	$^{13}C_4$-PFOS IS based	Average
PFNSW 003	ND	6,200	ND	ND	ND	6,200	7	7	7
PFNSW 004	ND	1,900	ND	ND	139	2,039	3	2	2
PFNSW DUP2	ND	3,860	91	75	118	4,144	4	3	3
PFNSW 005	ND	2,820	ND	320	243	3,383	2	1	2
PFNSW 012	ND	8,360	ND	97	248	8,705	8	6	7
PFNSW 014	ND	3,460	ND	ND	149	3,609	4	3	3
PFNSW 017	ND	11,900	76	2,440	4,620	19,036	12	11	12
PFNSW 018	ND	19,500	81	ND	54	19,635	17	13	15
PFNSW DUP1	ND	20,100	ND	ND	243	20,343	15	11	13
PFNSW 019	ND	5,630	ND	ND	240	5,870	4	3	3
PFNSW 020	ND	26,100	85	349	2,590	29,124	25	23	24
PFNSW 023	ND	74,800	ND	598	182	ND	39	26	33
PFNSW 025	ND	3,590	ND	77	ND	ND	3	3	3
PFTSW 001	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 002	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 003	685	1,890	ND	ND	ND	2,575	2	1	2
PFTSW 004	1,070	ND	ND	ND	ND	1,070	-	-	-
PFTSW 005	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 006	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 007	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 008	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 009	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 010	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW DUP2	9,980	220,000	2,930	3,270	3,050	239,230	132	113	122
PFTSW 011	ND	64,700	ND	ND	ND	64,700	46	31	38
PFTSW 012	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 014	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 015	ND	21,200	ND	ND	ND	ND	15	11	13
PFTSW DUP1	7,050	409,000	1,810	2,030	2,800	422,690	275	237	256
PFTSW 016	ND	ND	ND	ND	ND	0	-	-	-
PFTSW 017	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 018	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 019	ND	ND	ND	ND	ND	ND	-	-	-
PFTSW 020	ND	ND	ND	ND	ND	ND	-	-	-

D. Quality Assurance Discussion

The NTA (Section A) and semi-quantitation analysis (Section C) produced independent determinations of peak area for the compound ClPFPECA. Therefore, the peak areas for this compound in each sample (Table 10) are not expected to be the same as those reported for NTA analysis in Tables 4-6 (Chem. Ref. #11). However, we can treat peak areas determined in the two separate analytical procedures as laboratory replicates that provide an indicator of the reproducibility of laboratory analysis for at least this one compound.

Peak areas provided in the tables noted above do vary slightly, but they their values are very close as indicted by Figure 2 where the relationship between the sample peaks areas observed in NTA (Section A) and those determined in the semi-quantitation analysis (Section C) is shown. Data include the NTA raw peak areas before screening for reporting limit and the summed congener peak area for the semi-quantitation analysis.

The close relationship indicates very good reproducibility of peak area in laboratory analyses (Figure 2). The repeatability of sample replicates over the range of peak areas within the samples has an R^2 of 1. Two samples are exceptions and have been isolated from the group as discussed below.

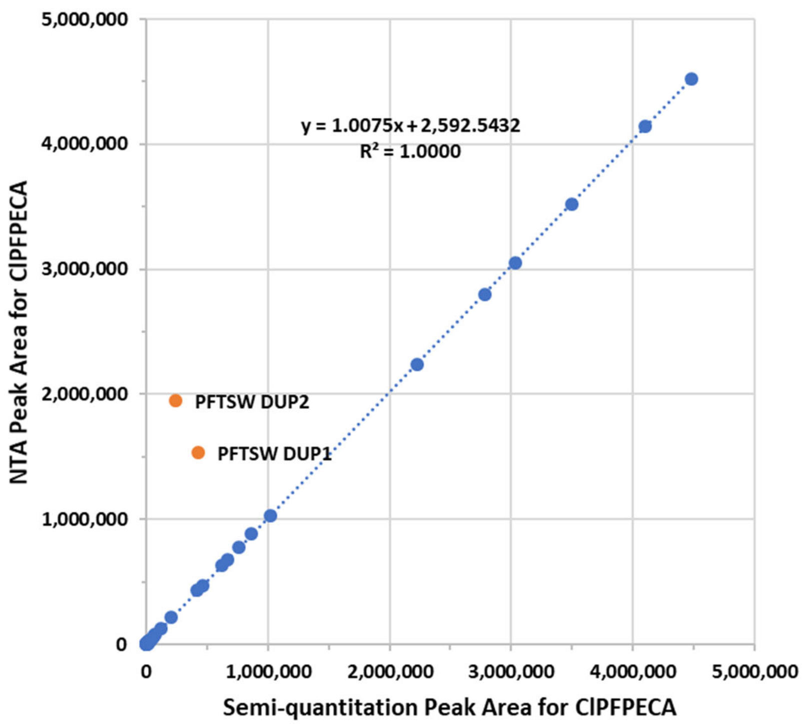

Figure 2. Peak area of ClPFPECA determined in the NTA analysis in relation to that determined in the semi-quantitation analysis.

An additional measure of the reproducibility of laboratory "replicates" can be calculated as the Coefficient of Variation (CV) of the two sample peak areas using equation 4:

Equation 4. Coefficient of Variation (CV) in % = (Standard Deviation Replicate Sample Peak Areas /Mean Replicate Sample Peak Areas) x 100.

The average CV for the 41 samples with detectable ClPFPECA peak areas in both samples was 13.9% and well within project goals of less than 50%[2].

The close relationship between peak areas in the two analyses also suggests that the normalization calculation used in NTA to align peak areas of samples with different injection volumes did so without introducing systematic error (Section A).

There are two outliers to the relationship shown in Figure 2 (PFTSW DUP1 and PFTSW DUP2). There were detectable levels of ClPFPECA in these two samples in both NTA and semi-quantitation analyses, but the values reported in NTA in Table 5 are significantly higher than expected based on the semi-quantitation results in Table 10. The differences in these two samples may reflect analytical procedures. Semi-quantitation is a more sensitive analysis and should be relied on when available.

Although we only have replicated analytical results for one compound (ClPFPECA), this result may provide information regarding the differences in peak areas that are evident in some duplicates that raise some question about the reliability of NTA results in Tables 3-6. The same similarities and discrepancies in peak areas that exist between the 9 duplicate samples that were discussed in Section A were also present in the semi-quantitation analysis in Section C. Sample duplicates that showed strong agreement in one analysis also showed strong agreement in the other analysis. Similarly, duplicates that showed strong disagreement in one analysis, also showed strong disagreement in the other analysis (e.g. Samples PFPW008 and DUP and samples PFPW012 and PFPWDUP1 in Table 3). Significant variation in results can be expected in NTA. However, within this dataset, assuming that estimating the abundance of ClPFPECA is reflective of other analytes, the similarity in duplicate results between analyses where peak area was independently determined suggests that most of the significant discrepancies between the duplicates probably exists within the samples rather than as a result of the NTA laboratory procedures.